Transport through small world networks

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We numerically investigate the transport properties through a system where small world networks are added to a one-dimensional chain. One-electron Green's function method is applied to standard tight-binding Hamiltonians on networks, modeled as (i) adding connections between any two nonadjacent random sites in the chain, (ii) introducing finite one-dimensional chains between any pair of such connected sites, and (iii) attaching finite dangling chains at random sites in the chain. Due to the small world bonds and dangling conduction paths, the systems have irregular geometrical shapes, leading to quenched disordered systems. We consider the qualitative influence of the small world bonds and dangling bonds on the transmittance and find that the systems exhibit a strong energy dependence on the transmittance, with strong sample-to-sample fluctuations. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2752142]

I. INTRODUCTION

Recently, small world network (SWN) models[1] have been a subject of intense interest as they are intermediate between regular lattices and random graphs. Many studies have been made of the scaling properties on small world systems,[2] percolation behavior,[3] localization-delocalization behavior[4] and multifractality properties[5] in disordered quantum small world models. SWNs have extensive uses in other areas as well; such as complex networks, communication networks, cellular networks, disease spreading, etc.

The transport in disordered systems has also been a subject of continuous interest for a long time. Based on Anderson's seminal paper[6] it was found that, in the absence of external symmetry breaking, all the eigenstates in disordered one- or two-dimensional systems are localized,[7,8] yielding nonmetallic states. A large effort concerning the electron transport has been devoted to the description of electron scattering from impurities in narrow wires.[9] Work has been done to develop and analyze model Hamiltonians which include different types of disorder: structural,[10,11] topological, compositional, orientational, etc.

In this article we focus on one issue, related to electron transmission, of how a SWN affects the transmittance. There are many materials exhibiting this type of disorder due to the randomness in their geometry: ramified fractals, percolation networks,[12–14] and branched polymers. We regard a SWN as small world (SW) connections or SW bonds (SWbs) of finite length. Our systems start with a uniform infinite one-dimensional (1D) chain, with a single transport channel, for which all allowed eigenstates are itinerant (extended) Bloch-type states. SWbs are then attached to a central portion of this chain in random configurations, leading to quenched geometrically disordered systems. In this theoretical work, we studied the electron transport on such systems by using a full quantum mechanical analysis at the one-electron level within the elastic regime.

It is known that for a perfect conducting channel without irregularities or scattering mechanisms, i.e., ballistic systems, the transmittance ($\mathcal{T}$) goes to unity and the conductance of an ideal 1D conductor becomes $G_c=\frac{e^2}{\pi\hbar}\mathcal{T}=\frac{e^2}{\pi\hbar}$,[15,16] being energy independent. Randomly placed point scatterers or geometry of the sample[17] cause spatial variations in the transmittance. Owing to the relative phases of the scattered waves, which may change with the Fermi energy, one may see complete or exponentially small transmittance. The variations in the transmittance or conductance are known as conductance fluctuations,[18] where $\mathcal{T}\rightarrow\mathcal{T}(E)$ exhibits strong fluctuations as a function of energy (E) of the electron.

The purpose of this article is to present some numerically obtained results concerning the behavior of the transmittance through SWbs. In Sec. II we introduce the model and the method; in Sec. III we present the numerical results for particular system configurations, and we give a summary in Sec. IV.

II. MODEL AND METHOD

We consider a 1D system of length L connected on both sides to reflectionless semi-infinite perfect wires acting as right and left leads (RL and LL, respectively). We used three models to analyze the transport properties of 1D systems related to SWbs. They all comprise of a perfect 1D chain with only one orbital per site i, $|i\rangle$, with on-site energy ε_1.

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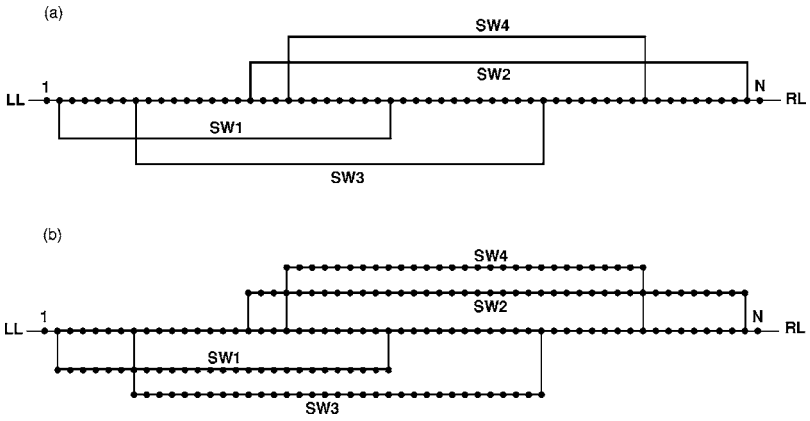

FIG. 1. Schematic picture of SW networks inserted in the main chain (a) for SWA, (b) for SWB, for a particular configuration: A chain with a length of N plus four SWbs. In both models, at most, one SWb is allowed at each site.

When only nearest-neighbor (NN) interactions are taken into account, with t_1 giving the NN hopping energy, the Hamiltonian takes the usual form,

$$H^{1D} = \varepsilon_1 \sum_i |i\rangle\langle i| + t_1(|i\rangle\langle i+1| + |i+1\rangle\langle i|). \tag{1}$$

In the first model (SWA) we attach to the chain SWbs by connecting two randomly chosen atoms with hopping energy t_2 [see Fig. 1(a)],

$$H^A = H^{1D} + t_2 \sum_j^{N_{SW}} (|i_j^1\rangle\langle i_j^2| + |i_j^2\rangle\langle i_j^1|), \tag{2}$$

where N_{SW} is the total number of SWbs, and i_j^1 and i_j^2 index the first and second sites in the 1D chain linked by the jth SWb, with $i_j^2 - i_j^1 > 1$.

The second model (SWB) is an extension of the former toward more realistic systems, in which atoms are now included along the SWbs;[19] see Fig. 1(b). If each atomic orbital (AO) within the jth SWb is denoted by $|k_j\rangle$, and assuming all of them have the same on-site energy ε_2 and the same NN interaction t_2, the Hamiltonian for the system takes the form

$$H^B = H^{1D} + \sum_j^{N_{SW}} [H^{SW_j} + t_2(|i_j^1\rangle\langle k_j^1| + |k_j^1\rangle\langle i_j^1| + |i_j^2\rangle\langle k_j^2| + |k_j^2\rangle\langle i_j^2|)], \tag{3}$$

where k_j^1 (k_j^2) denote the first (last) atoms in the jth SWb, and i_j^1 and i_j^2 now index the atoms in the chain linked to the SWb. H^{SW_j} is the Hamiltonian part associated with each SWb:

$$H^{SW_j} = \varepsilon_2 \sum_{k_j=k_j^1}^{k_j^2} |k_j\rangle\langle k_j| + t_2 \sum_{k_j=k_j^1}^{k_j^2-1} (|k_j\rangle\langle k_j+1| + |k_j+1\rangle\langle k_j|). \tag{4}$$

Thus SWB corresponds to segments of 1D tight-binding Hamiltonians added to make the SWbs, a process that leads to physical SWNs.[19]

Finally, our third model (SWC) adds dangles to the 1D lattice. The dangles are dangling dead-end bonds containing an arbitrary number of atoms. They are constructed by switching off the interactions between a randomly chosen pair of orbitals, $|k_j^0\rangle$ and $|k_j^0+1\rangle$, within a SWb of the second model (see Fig. 2),

$$H^C = H^B - \sum_j^{N_{SW}} t_2(|k_j^0\rangle\langle k_j^0+1| + |k_j^0+1\rangle\langle k_j^0|). \tag{5}$$

A common restriction to all of our models is that every atom in the main chain is connected to at most three atoms: two of them are the NNs in the 1D chain via t_1, and the other can be a SWb, through t_2. These models involve many parameters, namely, the t_2/t_1 ratio and the $\varepsilon_1 - \varepsilon_2$ on-site difference, the number of SWbs (N_{SW}), the length of each SWb ($N_j = k_j^2 - k_j^1 + 1$), its location with respect to the chain (i_j^1 and i_j^2), and the location of any dangle within each SWb (k_j^0).

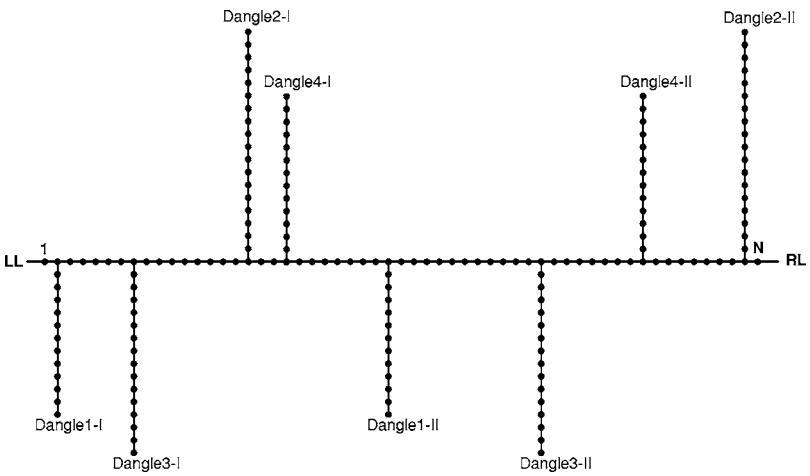

FIG. 2. Schematic picture of the system for SWC, for a particular configuration: A chain with a length of N plus four broken SWbs, i.e., eight dangles.

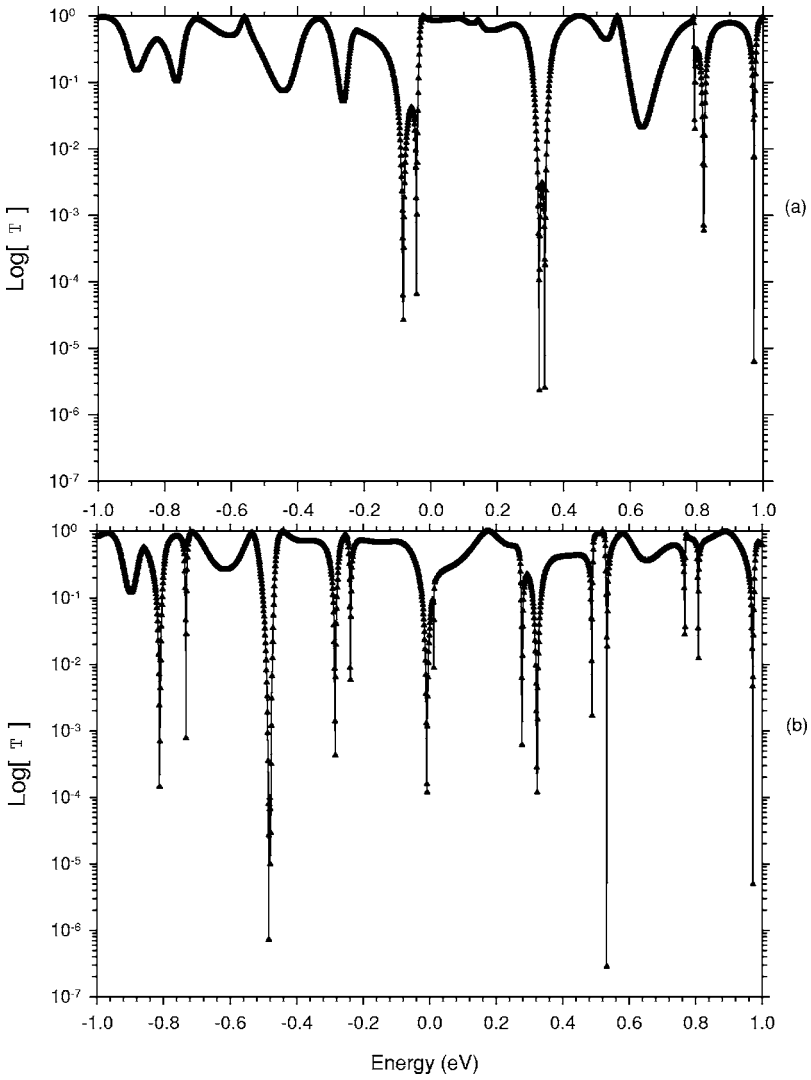

FIG. 3. Logarithm of the transmittance as a function of E for SWA in a system of length $L=100$ dressed with (a) four SWbs, (b) 10 SWbs (see text).

The transmittance for SWA, SWB, and SWC is evaluated within a one-electron Green's function formalism. To this end, the system is split into the so-called principal layers (PLs).[20] At the left and right bulklike leads, each PL contains just one atom, while the entire scattering region, comprising of the SWbs plus the 1D chain sites 1 through N (see Fig. 1), are all considered as a unique PL which we denote as s. The Green's function for the entire system is evaluated recursively employing the Green code;[21] first the Green's function for a semi-infinite 1D chain (surface) is trivially solved.[20] Next, the Green's function for the isolated PL s, $\mathcal{G}_{ss}(E)$, is calculated from its molecular orbitals,

$$\mathcal{G}_{ss}(E) = \sum_{m}^{M} \frac{|u^m\rangle\langle u^m|}{(E - E^m + i\delta)}, \tag{6}$$

where m denotes each molecular orbital (MO), M gives the number of atoms in PL s, E^m and $|u^m\rangle$ are the MO energies and eigenvectors, and δ is the imaginary part of the energy.

The scattering region is then coupled first to the left lead (LL) and next to the right lead (RL) by means of the Dyson equation.[20] The zero temperature transmittance for electrons traveling from left to right is then evaluated according to the following formula:[18]

$$\mathcal{T}(E) = \mathrm{Tr}[\mathcal{G}_{i+1,i}(E)\Gamma_i^l(E)\mathcal{G}_{i,i+1}^{\dagger}(E)\Gamma_{i+1}^r(E)], \tag{7}$$

where i refers to any PL in the system, $\mathcal{G}_{i+1,i}(E)$ denotes the Green's function linking PL i to the PL $i+1$ to its right, and $\Gamma_i^l(E)$ ($\Gamma_{i+1}^r(E)$) are the left (right) imaginary parts of the self-energies for PL i ($i+1$). Since we assume the system is in a steady state, $\mathcal{T}(E)$ is independent both of the PL index i and of the electron flow direction. Note that the breakup into PL is a computational tool to allow large-scale calculations, but does not affect the results which could be accomplished in principle using a brute-force calculation.

III. NUMERICAL RESULTS

Here we present numerical results for the transmittance of finite systems (connected to two semi-infinite leads) for each model, calculated at zero temperature, i.e., at the Fermi energy $E=E_F$ of the electrons (we ignore the spin of the electrons). In order to explore the transport properties, the transmittance is evaluated for different numbers of SWbs and dangles (hereafter SWbs is used to include dangles as well) connected to the main chain. Calculations were performed with on-site energies uniform in all parts (SWbs plus main chain) of the system and hopping terms are taken to be t_1

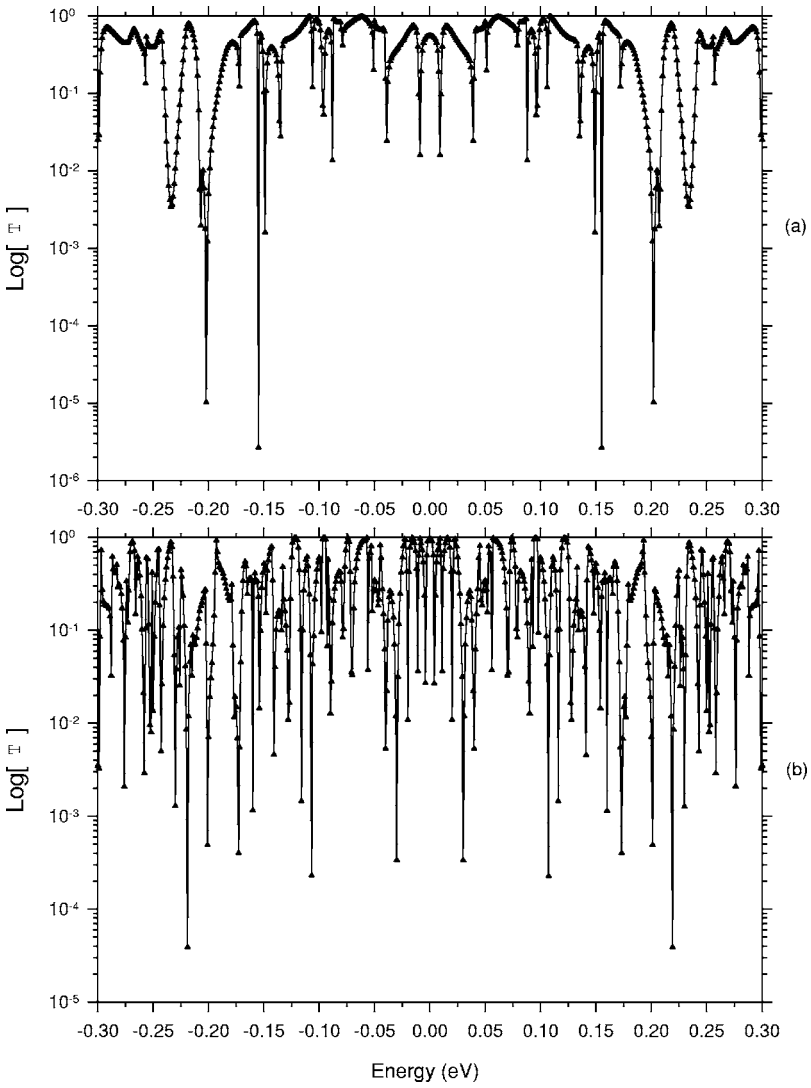

FIG. 4. Logarithm of the transmittance as a function of E for SWB in a system of length $L=100$ dressed with (a) four SWbs, (b) 10 SWbs (see text) in the expanded energy scale.

$=1.0=2t_2$. Since we are examining the effects of SWbs and, therefore, how the geometrical disorder affects the transport properties the standard diagonal disorder is ignored and the on-site energies are set to zero ($\varepsilon_1=\varepsilon_2=0$). The imaginary part of the energy was set to a small value, $\delta=0.001$ meV.

Given that there is no on-site disorder the transmittance is governed only by geometrical disorder, arising from randomly placed SWbs, rather than from variations of the length L of the system.[22] Hence, SWbs located at the same sites (same atoms) on the main chain of different lengths will result in exactly the same transmittance variation. Thus the length of the 1D chain is taken to be fixed and we mainly focus on how $\mathcal{T}(E)$ varies with randomly positioned SWbs. For this contemplation we, here, specifically present results for two systems each containing 100 sites, $L=100$, with four SWbs and 10 SWbs. The results of SWA, SWB, and SWC are displayed in Figs. 3–5, respectively. To exhibit extreme fluctuations explicitly Figs. 4 and 5 are illustrated on a different energy scale. Except for SWC, the variation in $\mathcal{T}(E)$ is found to depend significantly on the number and position of SWbs. For SWC the number of atoms on the dangles play the main role rather than the position of SWbs. Figures 4 and 5 have much narrower resonances and sharper maxima than Fig. 3, one reason of which is due to an increase in the scattering centers as a result of atoms on the SWbs. Depending on the path of the electrons, there are sharp fluctuations in $\mathcal{T}(E)$ induced by randomly placed SWbs which are operating incoherently. Attaching more randomly positioned SWbs on the main chain leads to additional enhancement of such fluctuations (making the width of the peaks narrower, varying the resonance locations, giving rise to progressively sharper peaks, and enhancing the number of peaks in a given energy interval). The resonances, taking place at fixed energies for each configuration, are inherent to the sample configuration (the location and number of the SWbs for each model). One can construe that the behavior of the resonances stems from the interplay between the number and random location of the SWbs for each model, i.e., the position and the thickness of the peaks depends strongly on the sample. However the qualitative aspects do not change substantially from sample to sample. The effects related to each model can be deduced from the relation of localization length $\mathcal{L}(E)$ and transmittance $\mathcal{T}(E)\propto\exp[-1/\mathcal{L}(E)]$.

It is seen that along with some energy values where $\mathcal{T}(E)$ is exponentially small there are certain energy values at which $\mathcal{T}(E)$ exhibits well pronounced maxima. For SWA there is no symmetry in energy. In this model, for $E<0$, only

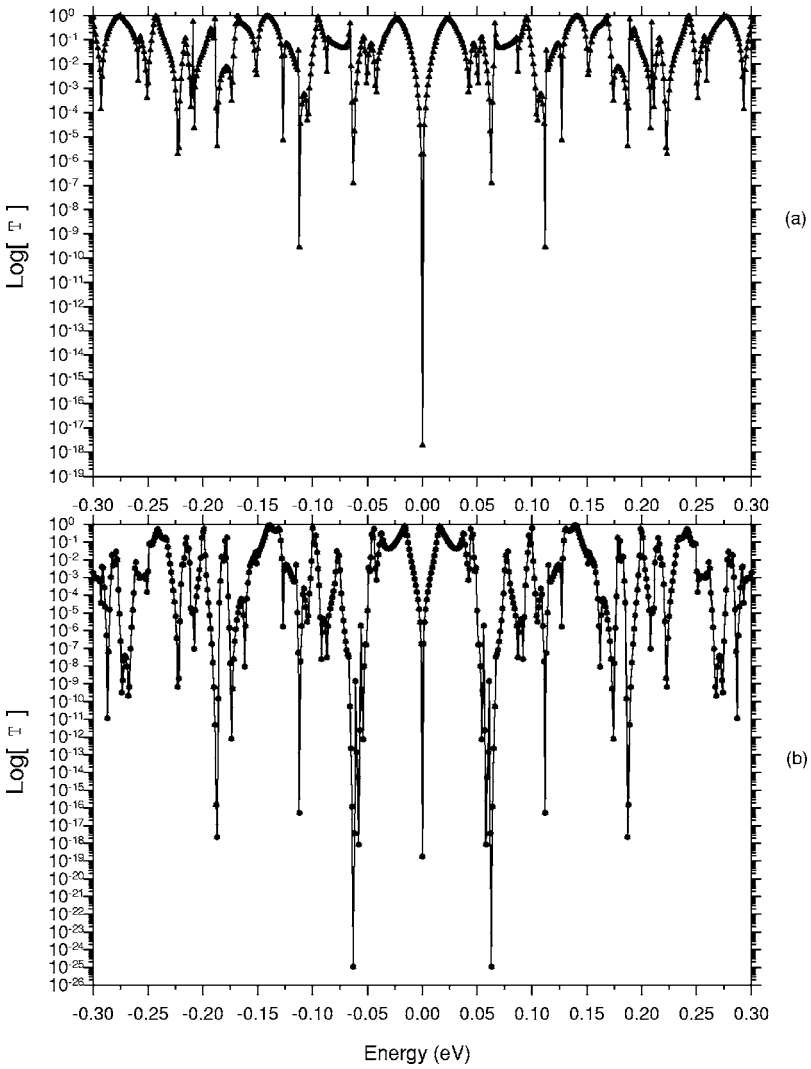

FIG. 5. Logarithm of the transmittance as a function of E for SWC in a system length of $L=100$, where (a) eight dangles and (b) 20 dangles were placed (see text) in the expanded energy scale.

those particles having resonant energies given by MO eigenenergies have more probability to get through the system. As a consequence, one may have sharp peaks and narrow resonances of the transmittance for $E<0$. For $E>0$ these peaks occur at energies away from the eigenvalues. The asymmetry in this model, where there are no atoms placed on SWbs, comes from the Hamiltonian. There is a symmetry in energy, $\mathcal{T}(E)=\mathcal{T}(-E)$, for SWB and SWC. It simply arises from the corresponding Hamiltonian, which has all on-site energies set to zero and there are no overlaps. Since the Hamiltonian has a particle-hole symmetry in these models the distribution of eigenenergies must be symmetric around $E=0$. The transmittance in these models has sharp dips at certain energies close to the MO energies. Maximum transmittance $[\mathcal{T}(E)\rightarrow 1]$ caused by the random location of the SWbs may enable the electrons to see an allowed band. A main general result for disordered systems is that the transmittance may go to zero[23] or deviate substantially from unity at particular energy values for each configuration. Specific systems may exhibit huge resonances as well, occurring at certain energies.[22,24] Therefore, the transmittance in our models can be characterized by the randomly distributed resonances leading to a strong dependence with the energy of the incoming particle.[24,25]

Finally, we also consider the effect of the hopping energy t_2 on the transmittance. We take two extreme limits, $t_2=0$ and $t_2=100$, together with intermediate ones. The numerical results for SWA (with 10 SWbs) and SWB (with four SWbs) are presented in Figs. 6 and 7, respectively. The $t_2=0$ case, simply analogous to that where there are no SWbs, results in unity in the transmittance. In the opposite limit, $t_2=100$, the SWbs behave like an impurity potential of finite width which becomes infinitely strong. Therefore the $\mathcal{T}(E)$ approaches to zero, together with some small peaks at particular energy values associated with each model and SWb arrangement, and will vanish for all energies for $t_2=\infty$. The derivation of the transmittance for the simplest case, main chain plus dangle containing only one atom, is given in the Appendix. The analytical expression of the transmittance for these similar systems can also be found elsewhere[20] (see, for example, Ref. 26 for a lattice under the δ function potentials).

IV. DISCUSSION AND CONCLUSIONS

We have investigated the transmittance of uncorrelated electrons through an ideal 1D chain dressed with SWbs, resulting in a geometrically disordered system. We have exam-

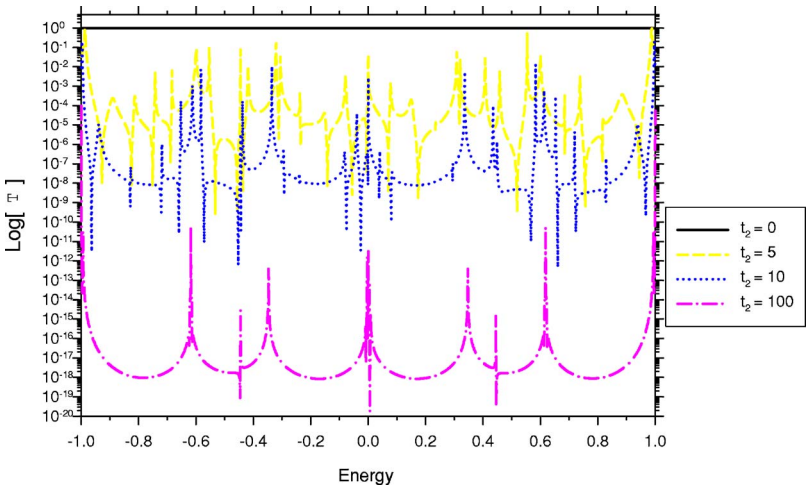

FIG. 6. (Color online) Logarithm of the transmittance as a function of E for SWA, for different t_2 values.

ined the effects of SWbs, distributed randomly, on the transmittance of a 1D tight-binding chain. The irregularity of the system originates from the geometry rather than from additional impurities. The width of the resonances and, so, the number of peaks changes by modifying the number and location of SWbs, as the scattering centers alter with such additions. However, the main qualitative features do not change significantly and do not differ qualitatively from the standard substitutional disorder.

Numerical results indicate that there is a strong energy dependence in the transmittance, which is the unusual case for systems with substitutional disorder. While for a ballistic case it shows the ideal behavior with a transmission of unity, the geometrical shape of the systems that we consider yields transmittance that are suppressed and deviate from unity or vanish[23] at some energies. By playing the number and the position of the SWbs, extended states may evolve into highly localized states with a modified number of transmission peaks. It causes a shift of the positions of the transmittance peaks, due to the energy dependence, and influences the character of the quantum transport. Thus transport in our systems may be directly compared with the transmission through systems with random potential steps or impurity potentials in a disordered medium, leading to the nonballistic situations (mean free path $l \leq L$). Since $\mathcal{T}(E)$ shows strong fluctuations as a function of E, and we have sample-specific random signals, this behavior can be ascribed to the phenomenon of the conductance fluctuations.[18] One remark is that the amplitude of the $\mathcal{T}$ modulation is subject to sample-to-sample fluctuations since $\mathcal{T}(E)$ depends on the details of nonballistic samples.

It was demonstrated that 1D chains of atoms and molecules can be set up.[27] Our model systems can be regarded as a model for percolation clusters,[28,29] and applied to the branched polymers, fractals or percolation networks, including other chainlike structures such as C chain, polymer's network formed by polymer chains, all atomic Au chain reconstructions on vicinal Si substrates, etc. These may all behave in a similar fashion. The atoms on the SWbs can be thought of as providing an effective potential on the chain, along which, it is distributed randomly. This is the case in the Anderson model where substitutional disorder is included rather than geometrical disorder. The dissimilarity between these two cases comes chiefly from the energy dependence of the effective potential in our models.

APPENDIX

For the sake of completeness we derive an explicit expression for the transmittance of a simple case of SWC. (The analytical expression for SWA and SWB then can be obtained similarly.) Here we consider the simplest case, where there is only one dangle containing one atom (see Fig. 8). For more complex cases the corresponding relations can be

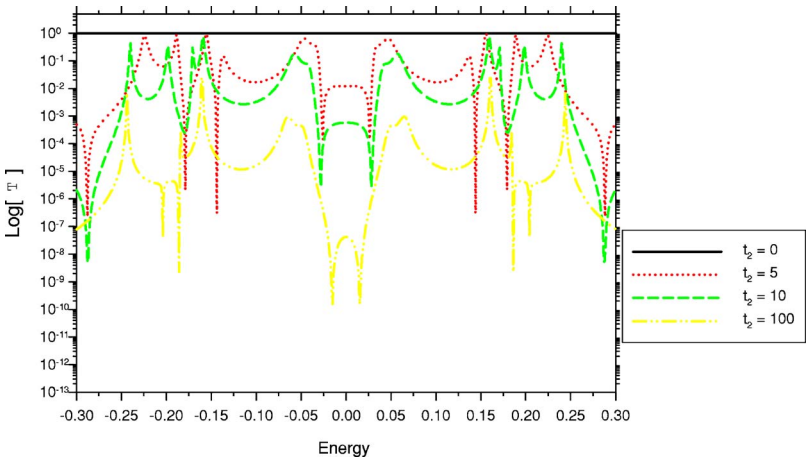

FIG. 7. (Color online) Logarithm of the transmittance as a function of E for SWB, for different t_2 values.

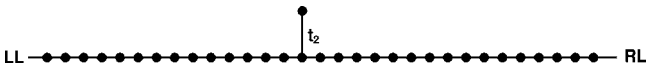

FIG. 8. Schematic picture of the model considered in the Appendix.

obtained with straightforward, but tedious, algebraic manipulations. Taking the scattering part, main chain plus dangle, as the perturbed part, the total ($\mathcal{G}$) and the bare ($\mathcal{G}_0$) Green's function can be related as $\mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\mathbf{t}_2$. It can be rewritten to yield the Dyson equation,

$$\mathcal{G}=\mathcal{G}_0+\mathcal{G}_0\mathbf{t}_2\mathcal{G}, \tag{A1}$$

where $\mathbf{t}_2$ is the perturbation potential given in the form

$$\mathbf{t}_2=t_2^{ij}+t_2^{ji}. \tag{A2}$$

Here site i refers to the main chain to which site j on the dangle is connected. Attaching these two adjacent sites one can find the matrix elements

$$\mathcal{G}^{ij}=0+\mathcal{G}_0^{ii}t_2^{ij}\mathcal{G}^{jj},$$

$$\mathcal{G}^{ji}=0+\mathcal{G}_0^{jj}t_2^{ji}\mathcal{G}^{ii},$$

$$\mathcal{G}^{ii}=\mathcal{G}_0^{ii}+\mathcal{G}_0^{ii}t_2^{ij}\mathcal{G}^{ji},$$

$$\mathcal{G}^{jj}=\mathcal{G}_0^{jj}+\mathcal{G}_0^{ji}t_2^{ij}\mathcal{G}^{jj}.$$

In a similar manner one can get the Green's function of any two sites on the main chain using the recursive relations iteratively. If we place the dangle between sites m and n on the main chain, then the corresponding total and bare Green's functions become $\mathcal{G}^{mn}$ and $\mathcal{G}_0^{mn}$, respectively. After obtaining a few sets of equations, the relationship between $\mathcal{G}^{mn}$ and $\mathcal{G}_0^{mn}$ is found to be

$$\mathcal{G}^{mn}=\mathcal{G}_0^{mn}+\frac{\mathcal{G}_0^{mi}t_2^{ij}\mathcal{G}_0^{jj}t_2^{ji}\mathcal{G}_0^{in}}{1-t_2^2\mathcal{G}_0^{ii}\mathcal{G}_0^{jj}}. \tag{A3}$$

Transmittance of the system is given by the expression $\mathcal{T}(E)=\frac{\mathcal{G}^{mn}}{\mathcal{G}_0^{mn}}$. Hence one needs to manipulate Eq. (A3) to obtain this ratio. The Green's function of any two sites for an unperturbed infinite chain (main chain) has the following form:[30]

$$\mathcal{G}_0^{kl}=\mathcal{G}_0^{ii}e^{I|k-l|\alpha}, \tag{A4}$$

where $\cos(\alpha)=\frac{E}{2t_2}$. The diagonal element of an infinite and finite chain (dangle) are given as $\mathcal{G}_0^{ii}=[E-2t_2\exp(I\alpha)]^{-1}$ and $\mathcal{G}_0^{jj}=\sin(\alpha)[t_2\sin(2\alpha)]^{-1}$,[30] respectively. Utilizing these definitions together with Eqs. (A4) and (A3), after some rearrangement, one finally finds the transmittance

$$\mathcal{T}(E)=\frac{\mathcal{G}^{mn}}{\mathcal{G}_0^{mn}}=\left(1+\frac{1}{4\sin^2(2\alpha)}\right)^{-1}=\frac{4t_2^2-E^2}{4t_2^2-E^2+t_2^4/E^2}. \tag{A5}$$

Hence, the transmittance decreases in terms of a hopping term as $\frac{1}{t_2^2}$.

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